Phase transitions and scaling laws in step bunching

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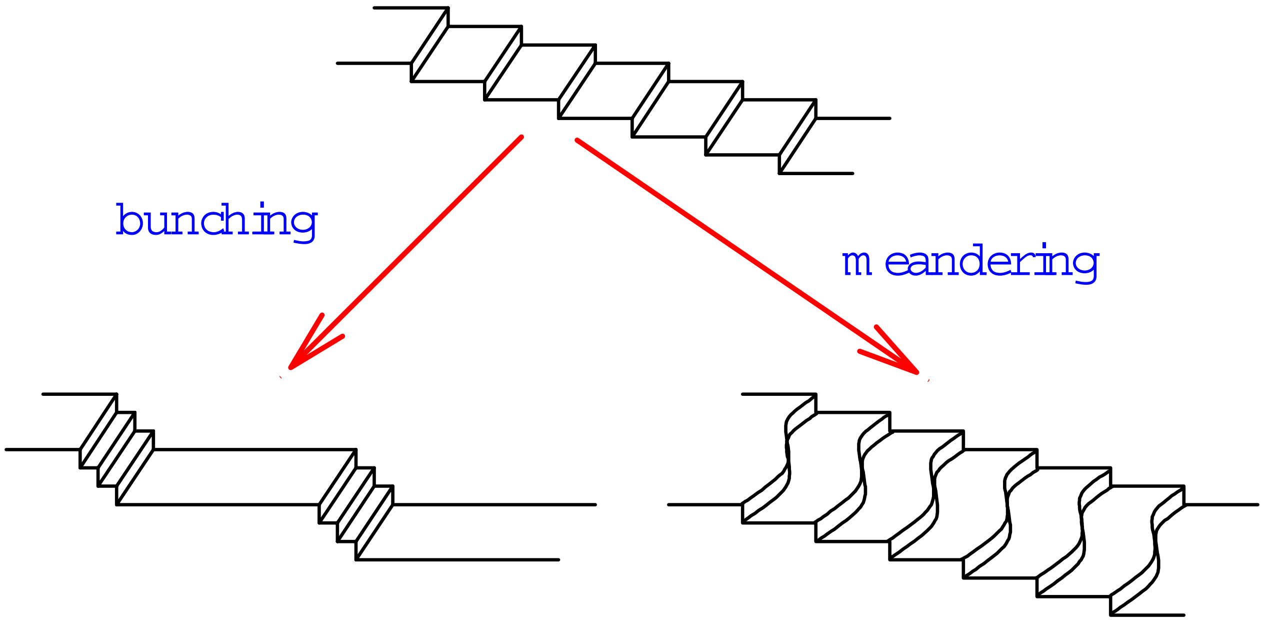


Discrete equations for steps dynamics

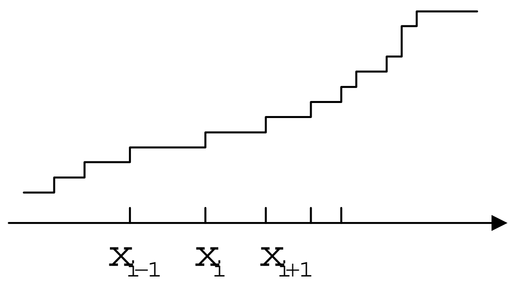
D.-J. Liu, J.D. Weeks '98

$$\frac{\partial x_i}{\partial t} = \frac{1-b}{2}(x_{i+1} - x_i) + \frac{1+b}{2}(x_i - x_{i-1}) + U(2f_i - f_{i-1} - f_{i+1})$$

Attachment/detachment-limited kinetics with Ehrlich-Schwoebel effect
electromigration under weak force

b **is the asymmetry of the attachment kinetics of adatoms (*Ehrlich-Schwoebel effect*)** $0 < b \leq 1$

is a measure of electromigration force (*electromigration*) $-\infty < b < \infty$



U **is a measure of step-step repulsion**

$$f_i = \left(\frac{l}{x_i - x_{i-1}}\right)^{n+1} - \left(\frac{l}{x_{i+1} - x_i}\right)^{n+1}, \quad n = 2$$

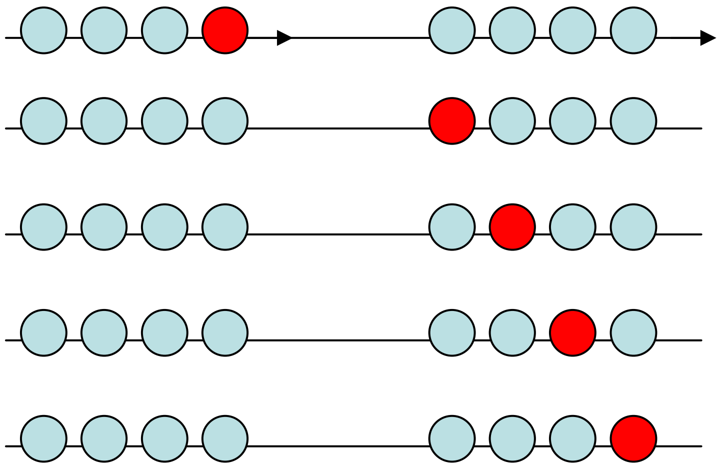
Bunching for wavelengths bigger than

$$M^* = 2\pi\left[\arccos\left(1 - \frac{bl}{12U}\right)\right]^{-1} \sim \sqrt{\frac{U}{b}}$$

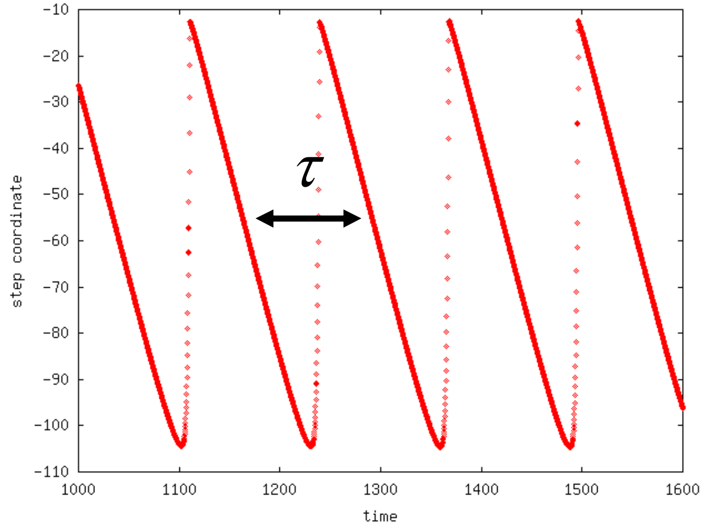
$\bar{l}$ **is an average terrace length** $\langle x_{i+1} - x_i \rangle$

Time scale associated with dynamics of steps

$$\frac{\partial x_i}{\partial t} = \frac{1-b}{2}(x_{i+1} - x_i) + \frac{1+b}{2}(x_i - x_{i-1}) + U \ldots$$



$M = 4$



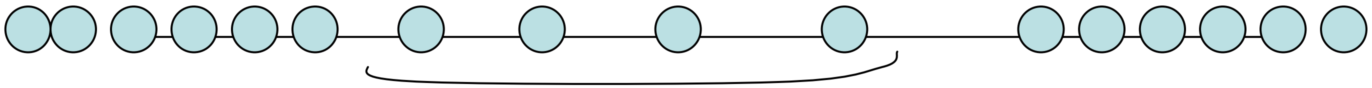
Targeted step trajectory

$$\Delta_j = x_{j+1} - x_j$$

$$\Delta_{j\pm 1}(t) = \Delta_j(t \pm \frac{\tau}{M})$$

Equation for a distance between two steps

$$\frac{d\Delta(t)}{dt} = \frac{1-b}{2}\Delta(t + \frac{\tau}{M}) + b\Delta(t) - \frac{1+b}{2}\Delta(t - \frac{\tau}{M}) + U(\ldots),$$



$b < 1$ **bunches**

Anzatz $\Delta(t) \sim \exp(qM\, t/\tau)$

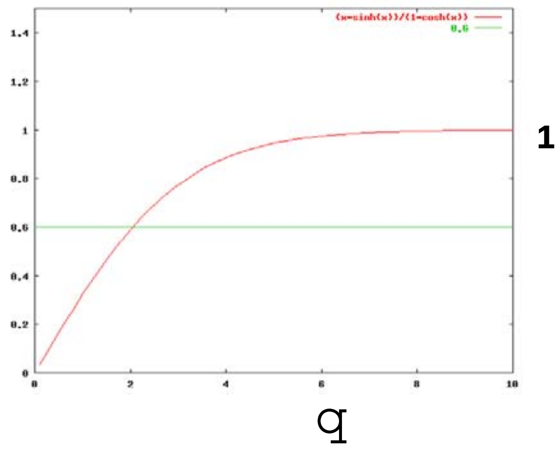
$\Delta_k / \Delta_{k-1} = \exp(q)$

$$b(\cosh(q) - 1) = \sinh(q) - qM/\tau$$

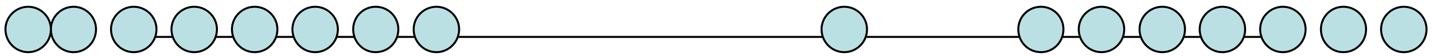
One can argue, that irrespective of the form of repulsion *[V.P., J. Krug, Europhys. Lett. 72, (2005)]*

$\frac{\tau}{M} \approx 1 + \frac{\kappa}{M}$ **for large bunch sizes**

$$b = \frac{q - \sinh q}{1 - \cosh q}$$

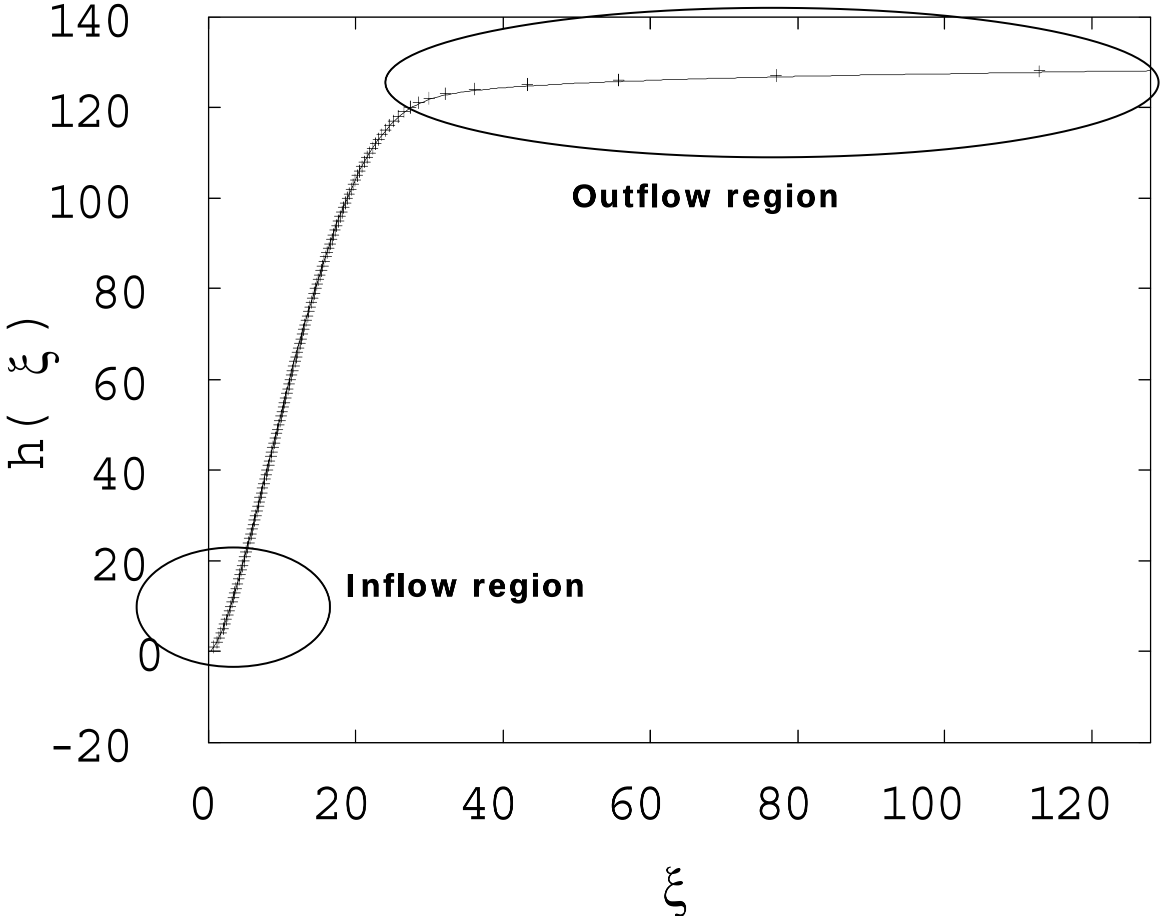


no solutions for $b > 1$



$b > 1$ **bunches**

Stationary bunch for b<1



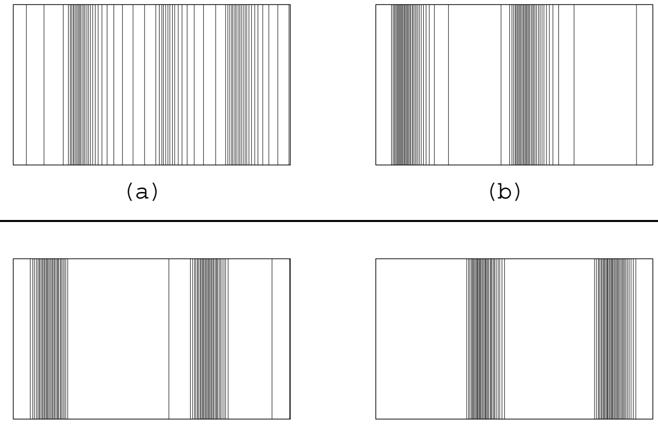
$b < 1$

Number of free steps N_f

$$l \exp[qN_f] \approx M l$$

$$N_f \approx \frac{\ln M}{q} \approx \frac{\ln M}{3b} \quad \text{when } b \leq 0.5$$

$b = 0.1$ $\quad$ $b = 0.5$



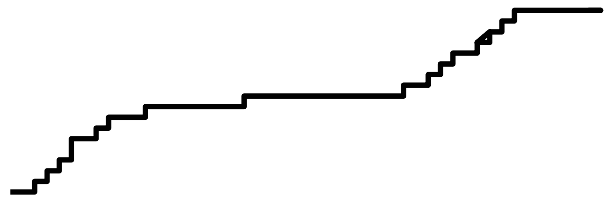
(a) (b) (c) (d)

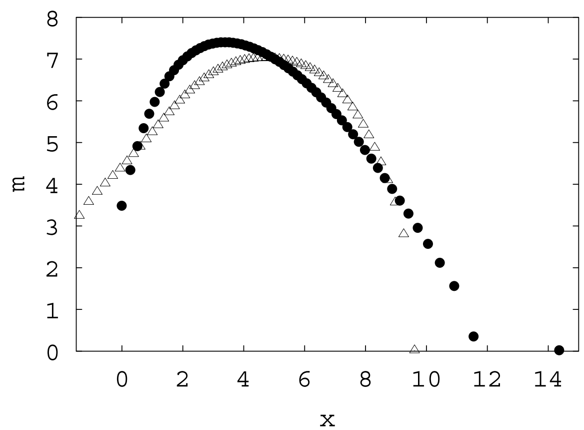
$b > 1$

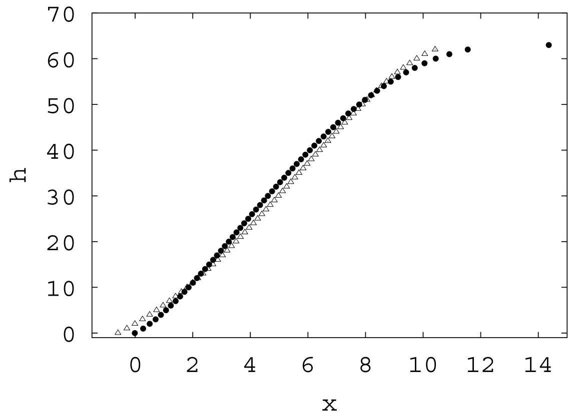
$$N_f = 0, 1$$

$b = 5$ $\quad$ $b = 20$

Cannon-like mechanism of step expulsion







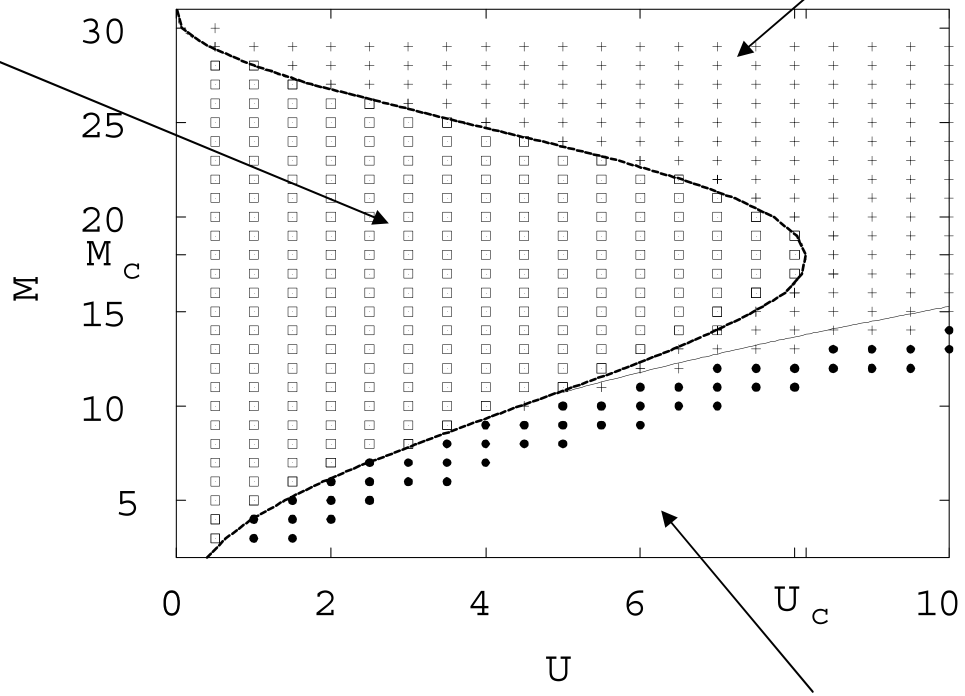
Regime without step expulsion
(dead zone)

$$M_c \approx 2.11 * b^{\frac{\alpha-1}{2}}$$

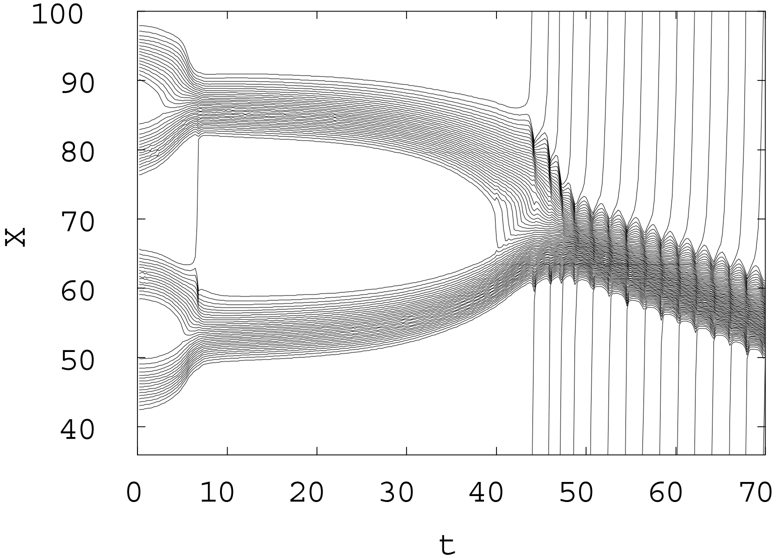
$$U_c \approx 0.01 * b^{\alpha};$$

$$\alpha \approx 2.87$$

steps exchange



no bunching

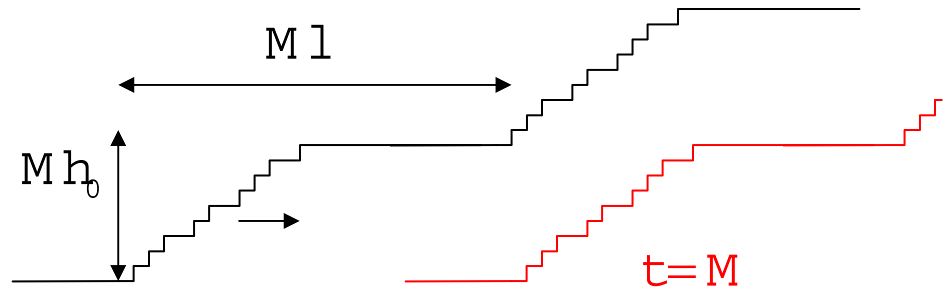


Mixed coarsening

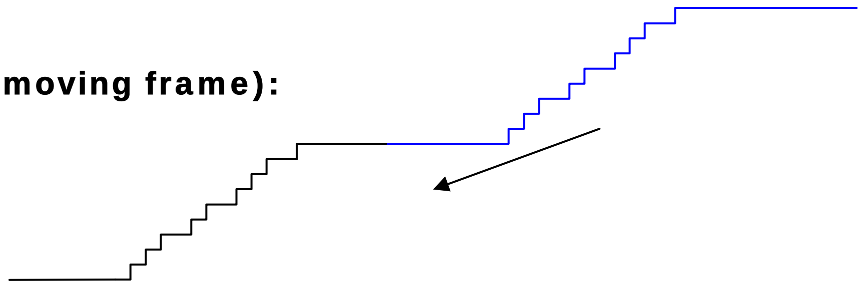
Bunch velocity

Individual step velocity $\left\langle \frac{dx_1}{dt} \right\rangle = l$

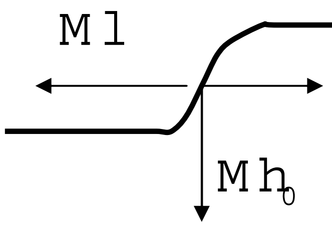
Without step exchange:



With step exchange (comoving frame):



After time τ **bunch shifts**



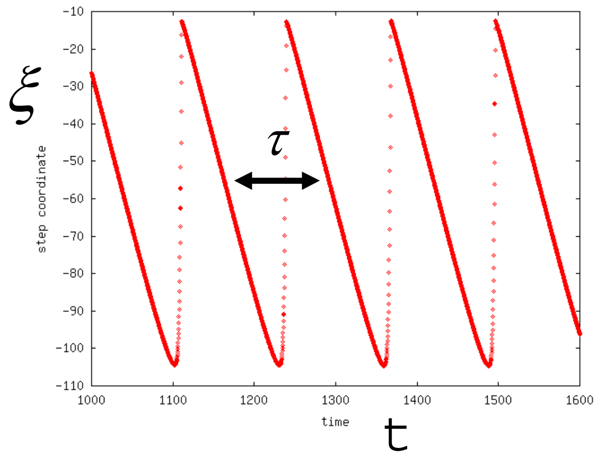
$$v = l\left(1 - \frac{M}{\tau}\right) \approx l\frac{\kappa}{M}$$

$$v_\perp = -h_0\frac{M}{\tau} \approx -h_0\left(1 + \frac{\kappa}{M}\right)$$

Moving bunches: scaling of bunch velocity

Equation for the stationary step trajectory

$$\frac{\partial \xi}{\partial t} = \frac{1-b}{2}\Delta(t) + \frac{1+b}{2}\Delta\left(t - \frac{\tau}{M}\right) - 1$$
$$+U\left(2f(t) - f\left(t - \frac{\tau}{M}\right) - f\left(t + \frac{\tau}{M}\right)\right) \quad .$$



Fourier transform $\quad \xi(t) = \sum C_n \exp(i w_n t), \qquad f(t) = \sum \Phi_n \exp(i w_n t)$

Extracting real part $\quad w_n = \frac{2\pi n}{\tau} = \sin(2\pi n/M) + 2U(1 - \cos(2\pi n/M)) \, \mathrm{Im}\left[\frac{\Phi_n}{C_n}\right]$

In the limit of $M \gg 1$

$$\frac{\tau}{M} = 1 + \frac{\kappa}{M} + O\left(\frac{1}{M^2}\right)$$

$$\kappa = -2\pi U \, \mathrm{Im}\left[n\Phi_n / C_n\right]$$

I. Chernov argument (1961) for a coarsening exponent

Velocity of a bunch with M steps $v \sim M^{-1}$

typical time for two bunches to merge $t \sim \frac{Ml}{v} \sim M^{2}$

typical bunch size growth as $M \sim t^{1/2}$

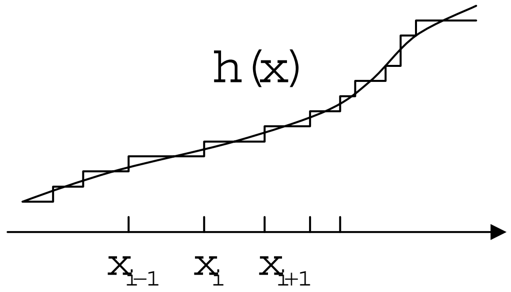
II. During evaporation of one monolayer, one step is emitted in average by every big bunch far enough from dead zone

Continuous equation for step bunches kinetics

J. Krug, '97

$$\frac{\partial h}{\partial t} + \frac{\partial}{\partial x}\left(-\frac{b}{2m} - \frac{1}{6m^3}\frac{\partial m}{\partial x} + \frac{3U}{2m}\frac{\partial^2 (m^2)}{\partial x^2}\right) = -1,$$

$$m(x,t) = \partial h / \partial x$$



An equation for a grown bunch in a periodic array of bunches is obtained by the Ansatz *[S. Stoyanov 2004]*

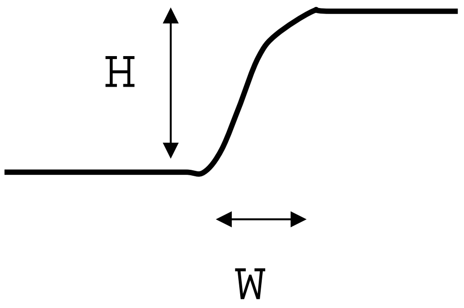
$$h(x,t) = h(x - vt) + v_{\perp} t$$

Integrating the resulting ODE, we obtain

$$\Omega\left(\xi + \xi_0 - h\right) + \frac{b}{2}\left(1 - \frac{1}{m}\right) - \frac{m'}{6m^3} + \frac{3U}{2m}(m^2)'' = 0$$

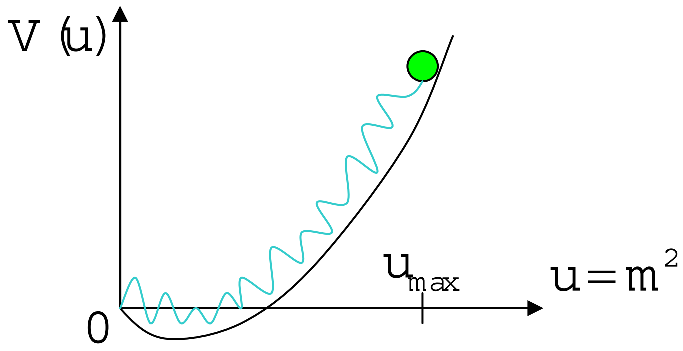
$$h(\xi + M\,l) = h(\xi) + M\,h_0$$

$$\Omega = 1 - \frac{M}{\tau}$$



$$W = H^{\gamma}$$

$$l_{min} = H^{\alpha}$$



$$\Omega\left(\xi + \xi_0 - h\right) + \frac{b}{2}\left(1 - \frac{1}{m}\right) - \frac{m'}{6m^3} + \frac{3U}{2m}\left(m^2\right)'' = 0$$

multiply by $m\left(m^2\right)'$

and integrate:

$$\left[\frac{3U}{4}\left(\left(m^2\right)'\right)^2 + b\left(\frac{m^3}{3} - \frac{m^2}{2}\right)\right]_a^c =$$

$$-2\Omega\int_a^c m^2 m'(\xi + \xi_0 - h)\,d\xi + \frac{1}{3}\int_a^c \frac{(m')^2}{m}\,d\xi$$

$$\int_0^{c_0}\left((m')^2/m\right)\,d\xi = \left[-m' - \left(36U m^2\right)^{-1}\right]_0^{c_0} \approx \left(36U\varepsilon^2\right)^{-1} = I_0$$

$$I_\Omega = 2\Omega\int_0^M m^2 m'\left(\xi + \xi_0 - h\right)\,d\xi \approx I_0/3$$

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Set $[a,c] \equiv \left[0,\ c_0\right]$, where $m(0) = \varepsilon$, $m(c_0) = m_{max}$

$$b m_{max}^3 \approx (1-\gamma) I_0$$

$$\gamma = \lim_{M\to\infty} \frac{I_\Omega\left[0,\ c_0\right]}{I_\Omega\left[0,\ M\right]} \approx 0.7 \pm 0.01$$

$$m_{max}^{-1} = l_{min} \approx \left(\frac{36U\varepsilon^2 b}{1-\gamma}\right)^{1/3} \sim \varepsilon^{2/3}$$

$$\varepsilon = \min m(\xi)$$

Moving bunches: scaling

(A) size of the first terrace in the bunch $$l_1 \approx (6U\varepsilon)^{1/3}.$$

(B) size of the minimal terrace in the bunch $$m_{max}^{-1} = l_{min} \approx \left(\frac{36U\varepsilon^2 b}{1-\gamma(b,U)}\right)^{1/3}$$ $\gamma \approx 0.7 \pm 0.01$

(C) Width of the bunch. $$W = \frac{Q^{-1}M}{6(1-\gamma(b,U))^{4/3}}\left(36U\varepsilon^2 b\right)^{1/3}$$ $Q \approx 0.323$

$$\varepsilon = \min m(\xi) = 1/l_{max}$$ **is defined microscopically as the inverse size of the *largest plateau* between two consecutive bunches**

In the leading order, scalings are consistent with

J. Krug, V. Tonchev, S. Stoyanov and A. Pimpinelli, Phys. Rev. B 71, 045412 (2005)

Summary

- We show existence of dynamic phase transition at critical value of electromigration force
- We predict mixed coarsening regime, with and without steps emission
- A new scaling parameter, size of the largest plateau emerges, in terms of which other bunch characteristics are expressed.
- We find:

(a) velocity of the bunch generically scales as the inverse distance between the bunches

(b) the surface height grows logarithmically in the outflow region between the bunches (for b<1)